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Conformational Dependence of Molecular Surface Electrostatic Potentials

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# CONFORMATIONAL DEPENDENCE OF MOLECULAR SURFACE ELECTROSTATIC POTENTIALS

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## Abstract

In a series of earlier studies, we have shown that a variety of solution, liquid and solid phase properties can be represented analytically in terms of quantities related to the electrostatic potentials on molecular surfaces. These quantities include the positive and negative extrema, the positive and negative average values and variances, and the average deviation. We have now investigated how sensitive these quantities are to the molecular conformation. Surface potentials were computed at the HF/6-31G\* level for a total of 35 conformations of ten different molecules. Our overall conclusion is that conformational effects upon applications of molecular surface electrostatic potentials are most likely to be of concern if (a) formation of the conformer considerably diminishes internal polarity, and/or (b) the application in question is strongly dependent upon the positive variance.

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## Introduction

The electrostatic potential  $V(\mathbf{r})$  created in the space around a molecule by its nuclei and electrons is well established as a guide to molecular reactive behaviour. (For reviews, see refs. [1-6].) It is defined by eq. (1), in which the molecule is treated as a collection of stationary point charges, the nuclei, surrounded by a continuous but static distribution of electrons:

$$V(\mathbf{r}) = \sum_A \frac{Z_A}{|\mathbf{R}_A - \mathbf{r}|} - \int \frac{\rho(\mathbf{r}') d\mathbf{r}'}{|\mathbf{r}' - \mathbf{r}|} \quad (1)$$

$Z_A$  is the charge on nucleus A, located at  $\mathbf{R}_A$ , and  $\rho(\mathbf{r})$  is the electronic density function of the molecule. The first term on the right side of eq. (1) is the nuclear contribution to  $V(\mathbf{r})$ , and is positive; the second term is due to the electrons and is accordingly negative.

Over a period of many years, the electrostatic potential was used extensively as a tool for identifying and ranking the molecular regions most susceptible to electrophilic and/or nucleophilic attack and for determining general patterns of positive and negative potential that promote or inhibit molecular interactions, such as those between drugs and receptors. Bernard and Alberte Pullman and their collaborators were pioneers in applying the electrostatic potential to the analysis of particularly biochemical systems; some of their numerous contributions are discussed in refs. [2-4]. The quantitative analysis of  $V(\mathbf{r})$  initially emphasized locating and evaluating the most negative potentials,  $V_{\min}$ . These are usually associated with (a) the more electronegative atoms, such as N, O, F, Cl, S and Br, and (b) unsaturated, aromatic and strained carbon-carbon bonds. The magnitudes of the  $V_{\min}$  can often be related to reactive properties, for instance the  $pK_a$  values of azine nitrogens [5], and epoxide carcinogenicity [4]. More recently, attention has focused upon the electrostatic potential  $V_S(\mathbf{r})$  on the molecular surface. It was shown that both the positive and negative surface extrema,  $V_{S,\max}$  and  $V_{S,\min}$ , can be related to reactive behavior. For example,  $V_{S,\max}$  and  $V_{S,\min}$  for a large variety of molecules correlate with hydrogen bond acidity and basicity, respectively [7]. (We take the molecular surface to be the 0.001 au contour of the electronic density, as suggested by Bader *et al* [8]. We have earlier discussed the use of  $\rho(\mathbf{r})$  contours to define molecular surfaces [9,10].) This approach was still limited in scope however;  $V_{\min}$ ,  $V_{S,\min}$  and  $V_{S,\max}$  are certainly key

features of the molecular electrostatic potential, but these site-specific quantities do not convey all the information that is contained in  $V(\mathbf{r})$ .

Accordingly, in recent years we have sought to develop mechanisms for more adequately describing and quantitatively characterizing the electrostatic potential over an entire molecular surface. We have found that this can be achieved through the introduction of several statistically-defined global quantities that explicitly reflect the magnitude of  $V_S(\mathbf{r})$  at each point on the molecular surface [11-14]:

- (a)  $\bar{V}_S^+$ ,  $\bar{V}_S^-$  and  $\bar{V}_S$  are the positive, negative and overall average potentials on the surface.

$$\bar{V}_S^+ = \frac{1}{n} \sum_{i=1}^n V_S^+(\mathbf{r}_i) \quad (2)$$

$$\bar{V}_S^- = \frac{1}{m} \sum_{i=1}^m V_S^-(\mathbf{r}_i) \quad (3)$$

$$\bar{V}_S = \frac{1}{m+n} \left[ \sum_{i=1}^n V_S^+(\mathbf{r}_i) + \sum_{i=1}^m V_S^-(\mathbf{r}_i) \right] \quad (4)$$

- (b)  $\Pi$  is the average deviation of  $V_S(\mathbf{r})$ ,

$$\Pi = \frac{1}{m+n} \sum_{i=1}^{m+n} |V_S(\mathbf{r}_i) - \bar{V}_S| \quad (5)$$

which we interpret as a measure of the local polarity, or internal charge separation, that is present even in molecules with zero dipole moment.

- (c)  $\sigma_+^2$ ,  $\sigma_-^2$  and  $\sigma_{\text{tot}}^2$  are the positive, negative and total variances of  $V_S(\mathbf{r})$ , which reflect the range or variability of  $V_S(\mathbf{r})$ , emphasizing its extrema,

$$\sigma_+^2 = \frac{1}{n} \sum_{i=1}^n [V_S^+(\mathbf{r}_i) - \bar{V}_S^+]^2 \quad (6)$$

$$\sigma_-^2 = \frac{1}{m} \sum_{i=1}^m [V_S^-(\mathbf{r}_i) - \bar{V}_S^-]^2 \quad (7)$$

$$\sigma_{\text{tot}}^2 = \sigma_+^2 + \sigma_-^2 \quad (8)$$

- (d)  $v$  indicates the degree of balance between the positive and negative surface potentials,

$$v = \frac{\sigma_+^2 \sigma_-^2}{(\sigma_{\text{tot}}^2)^2} \quad (9)$$

When  $\sigma_+^2 = \sigma_-^2$ , then  $v$  achieves its maximum possible value of 0.25.

In a series of studies, we have demonstrated that it is possible to develop quantitative analytical relationships of good accuracy for a variety of solution, liquid and solid phase properties in terms of some subset of these quantities (plus  $V_{\text{min}}$ ,  $V_{\text{S,max}}$  and  $V_{\text{S,min}}$ ), which are computed for the individual, isolated molecules. These properties include heats of fusion [15], vaporization [11] and sublimation [16], solubilities [17-19], solvation free energies [20,21], boiling points and critical constants [22], partition coefficients [23,24], diffusion coefficients [25], surface tensions [15], lattice energies [26], liquid and solid densities [15], and impact sensitivities [27].

In calculating the quantities defined by eqs. (1)–(9), our first step is to optimize the molecular geometry, so that we are presumably dealing with the most stable conformation. An important and frequently-posed question concerns the sensitivity of the computed quantities (and subsequent relationships) to the conformation of the molecule. How much is the surface electrostatic potential affected if the molecule is induced to adopt another conformation, perhaps due to thermal or environmental factors? Our objective in the present work has been to address this question.

### Procedure and Results

For the molecules **1–10**, we have investigated the conformations shown in Figures 1 and 2. Each molecular geometry was first fully optimized in the ground state, and then re-optimized in one or more different conformations (local minima). All calculations were carried out with Gaussian 92 [28] at the HF/6-31G\* level. For each conformation, we computed the surface area,  $V_{\text{S,max}}$  and  $V_{\text{S,min}}$ , and the properties defined by eqs. (2)–(9). The results are listed in Table 1, along with the HF/6-31G\* relative energies within each conformer group.

<chem>CH3-CH3</chem> <b>1</b>	<chem>CH3-CH2F</chem> <b>2</b>	<chem>CH3-CH2NO2</chem> <b>3</b>	<chem>CH3-CH2OH</chem> <b>4</b>	<chem>CH2Cl-CH2F</chem> <b>5</b>
<chem>CH2NH2-CH2NO2</chem> <b>6</b>	<chem>CH2OH-CH2OH</chem> <b>7</b>	<chem>CH3-CH2-CH2OH</chem> <b>8</b>	<chem>CH2=CH-COOH</chem> <b>9</b>	<chem>NH=CH-CH2NO</chem> <b>10</b>

## Discussion

### *Ethane and Its Monosubstituted Derivatives*

Both the staggered and the eclipsed conformer have been examined for molecules 1-4. The latter is invariably the less stable, by approximately 3 - 4 kcal/mole. (The experimental value for ethane is 3.0 kcal/mole [29].) The computed properties tend to be quite similar for each pair of conformers. In the case of 4, we also considered the structure (4c) resulting from a 64° rotation around the C-O bond of the staggered form. This requires an energy of only 0.1 kcal/mole, but produces a rather large change in the global property  $\bar{V}_S^-$ , indicating its sensitivity to the precise juxtaposition of the hydroxyl and neighboring hydrogens.

### *1,2-Disubstituted Ethanes*

Four conformers were investigated for each disubstituted ethane. The least stable structure is usually that in which the two substituents are eclipsed; 8c is an exception, presumably due to the short distance (1.95 Å) between one of the methyl hydrogens and one on the substituted carbon. In terms of our present objective, it is 5d that is of particular interest, in that it differs significantly from its conformers in terms of nearly *all* of its computed surface properties. This is not observed for any other of the disubstituted ethanes. In 5a, 5b and 5c, the negative halogen potentials evidently overlap and reinforce each other, creating a relatively strong negative region and a corresponding positive one. In 5d, on the other hand, the negative regions are separate and therefore weaker. The magnitudes of  $\Pi$  confirm that 5d has much less internal polarity than do its conformers. For 6 - 8, the surface properties generally tend to be fairly similar among the conformers. The most striking exceptions to this are  $\sigma_+^2$ ,  $\sigma_-^2$  for 8a and  $\bar{V}_S^-$  for 8b.

### *Molecules 9 and 10*

The four conformers of 9 fall neatly into two groups; 9a and 9c are significantly less stable than 9b and 9d, presumably because of the proximity of the hydrogens in the former, which creates considerable internal polarity. The surface properties are fairly

uniform within the two groups. Six different conformers of **10** have been investigated. Overall, they do not vary markedly in their surface properties.

### Summary

From the data in Table 1, certain generalizations can be made concerning the effects of conformational changes upon the molecular surface properties of present interest:

- (a) The surface areas are only slightly affected.
- (b) The two site-specific properties,  $V_{S,max}$  and  $V_{S,min}$ , and the global properties  $\bar{V}_S^+$  and  $\Pi$  usually change relatively little. The only exceptions to this are **5d** and the pair **9a/9c**, which were formed by rotations that either eliminated or produced regions of markedly reinforced negative or positive potential. This is then reflected in all of the properties of  $V_S(\mathbf{r})$ . However increasing the internal polarity can normally be expected to significantly decrease molecular stability, so that conformers such as **9a** and **9c** are less apt to play important roles.
- (c)  $\sigma_+^2$  is the most sensitive to conformational variations. It is probable that  $\sigma_{tot}^2$  and  $v$  will consequently be affected, although perhaps not to the same extent because they also include  $\sigma_-^2$ .

On the basis of the results in Table 1, therefore, it appears that conformational effects upon applications of molecular surface electrostatic potentials are most likely to be of concern if

- (a) formation of the conformer considerably diminishes internal polarity, and/or (b) the application in question is strongly dependent upon  $\sigma_+^2$ .

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Molecule	Relative Energy	Surface Area	(kcal/mole)					(kcal/mole) <sup>2</sup>			ν	(kcal/mole)	
			V <sub>S</sub> <sup>+</sup>	V <sub>S</sub> <sup>-</sup>	Π	σ <sub>+</sub> <sup>2</sup>	σ <sub>-</sub> <sup>2</sup>	σ <sub>tot</sub> <sup>2</sup>	V <sub>S,max</sub>	V <sub>S,min</sub>			
1a	0.0	81.5	2.77	-1.45	2.15	3.28	0.62	3.88	0.135	6.2	-2.7		
1b	3.6	81.0	3.19	-1.49	2.41	3.42	0.59	4.01	0.125	6.5	-2.7		
2a	0.0	85.5	9.26	-17.93	11.08	19.6	90.2	109.8	0.147	20.0	-28.0		
2b	3.6	85.3	9.08	-18.49	10.96	22.7	88.0	110.7	0.163	20.4	-28.3		
3a	0.0	108.4	18.12	-22.37	19.32	42.4	83.6	126.0	0.223	30.9	-36.3		
3b	3.5	108.8	18.27	-22.52	19.47	43.6	82.7	126.2	0.226	30.7	-36.3		
4a	0.0	90.4	9.59	-14.32	11.28	100.6	169.5	270.1	0.234	47.4	-39.6		
4b	3.1	92.7	11.05	-14.14	12.05	98.0	161.9	259.9	0.235	48.7	-38.4		
4c	0.1	90.4	9.54	-19.37	11.55	86.6	172.0	258.7	0.223	47.1	-40.2		
5a	0.8	105.1	18.32	-14.12	16.24	57.4	42.5	99.9	0.244	32.6	-27.3		
5b	7.8	104.5	18.93	-15.85	17.41	59.0	56.0	115.0	0.250	35.8	-32.8		
5c	0.8	105.1	18.31	-14.12	16.23	57.3	42.5	99.8	0.245	32.6	-27.3		
5d	0.0	105.2	14.00	-10.20	12.15	30.6	26.3	56.9	0.249	21.8	-20.1		
6a	0.0	122.4	21.00	-19.29	19.90	87.0	79.1	166.1	0.249	38.7	-33.8		
6b	4.2	121.4	20.27	-18.95	19.32	68.4	78.2	146.6	0.249	35.4	-33.1		
6c	0.1	122.1	21.09	-19.17	19.87	91.8	80.3	172.1	0.249	39.5	-33.4		
6d	1.0	124.7	22.17	-20.04	20.81	115.6	84.6	200.0	0.244	43.2	-35.1		
7a	0.0	101.2	14.86	-18.61	16.06	135.5	131.4	266.9	0.250	55.0	-39.7		
7b	2.9	101.0	17.29	-21.58	18.28	114.5	114.2	228.7	0.250	48.6	-36.4		
7c	1.0	101.0	16.33	-19.56	16.97	138.4	123.0	261.4	0.249	55.3	-38.1		
7d	2.1	101.6	17.00	-18.14	17.33	188.5	134.6	323.1	0.243	54.0	-37.7		
8a	0.1	110.8	9.16	-11.27	9.95	96.9	123.1	219.0	0.249	49.0	-37.6		
8b	0.6	110.7	8.88	-19.81	10.15	64.2	168.5	232.7	0.200	47.1	-40.1		

(continued)

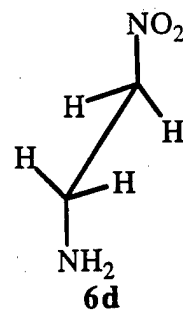
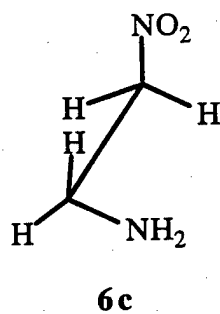
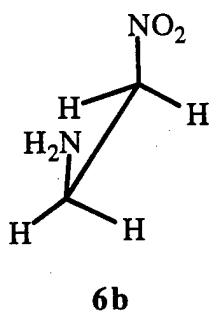
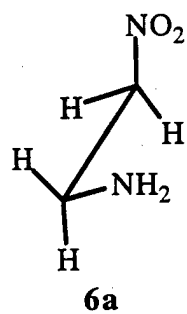
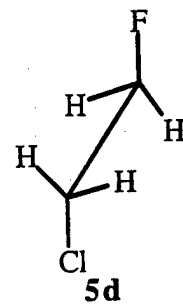
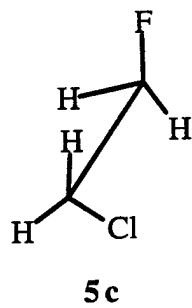
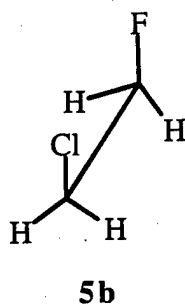
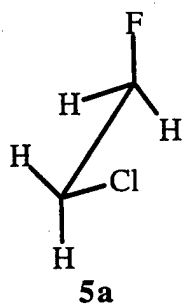
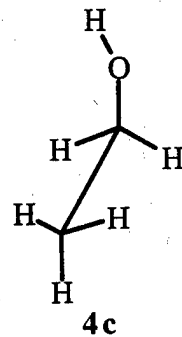
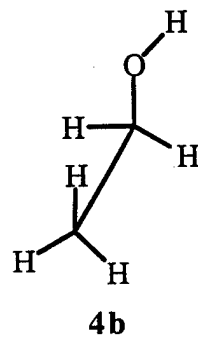
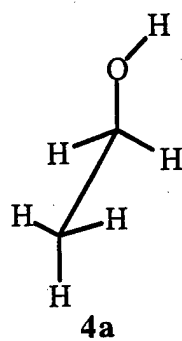
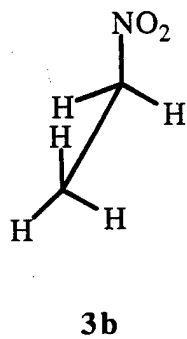
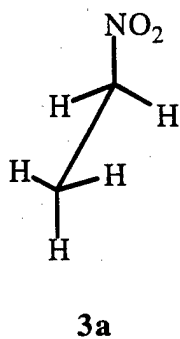
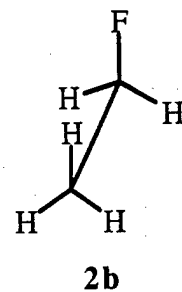
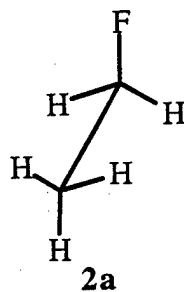
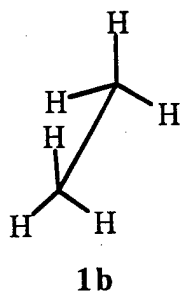
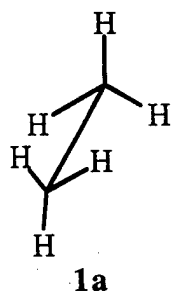
Table 1. Computed surface electrostatic potential quantities for conformers of 1-10 (continued).

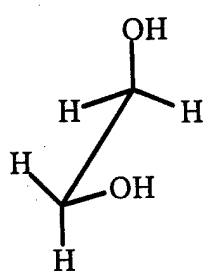
Molecule	Relative Energy (kcal/mole)	Surface Area (Å <sup>2</sup> )	$\bar{V}_S^+$	$\bar{V}_S^-$	$\Pi$	$\sigma_+^2$	$\sigma_-^2$	$\sigma_{tot}^2$	$\nu$	$V_{S,max}$	$V_{S,min}$
			(kcal/mole)		(kcal/mole) <sup>2</sup>						
8c	13.7	113.1	9.42	-12.91	10.40	84.9	166.1	251.0	0.224	48.3	-39.0
8d	0.0	111.7	8.23	-15.29	9.90	83.5	173.1	256.6	0.220	48.6	-39.6
9a	7.5	105.2	19.54	-24.29	21.28	212.0	211.0	423.0	0.250	70.3	-46.7
9b	0.0	105.5	13.25	-15.94	14.35	121.1	143.7	264.8	0.248	56.1	-38.1
9c	9.0	105.3	19.40	-27.08	21.56	191.1	162.1	353.2	0.248	69.3	-45.8
9d	0.5	105.5	13.39	-16.06	14.39	125.3	167.9	293.2	0.245	56.8	-39.5
10a	0.6	110.7	17.51	-15.11	16.23	83.3	66.5	149.8	0.247	38.8	-33.8
10b	2.8	110.5	19.34	-15.27	17.28	98.3	82.8	181.1	0.248	42.3	-37.7
10c	0.0	110.5	17.53	-15.56	16.43	84.1	70.7	154.8	0.248	38.4	-35.0
10d	2.0	110.3	19.46	-15.44	17.39	97.4	86.8	184.2	0.249	40.6	-38.4
10e	0.3	108.8	17.87	-15.31	16.56	73.8	71.8	145.6	0.250	36.4	-35.0
10f	2.9	108.9	20.88	-16.26	18.61	104.0	93.8	197.8	0.249	41.4	-40.1

## Figure Captions

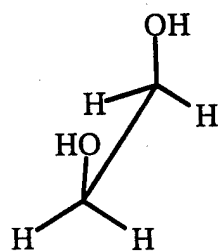
Figure 1. Conformers investigated for molecules **1 - 6**.

Figure 2. Conformers investigated for molecules **7 - 10**.

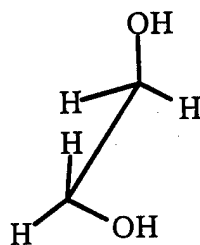




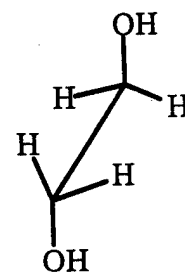
7a



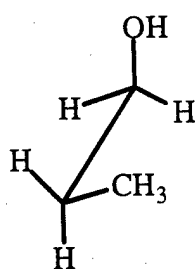
7b



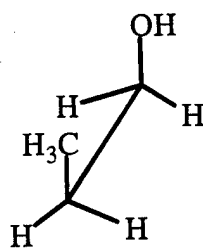
7c



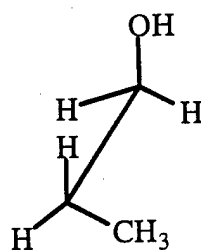
7d



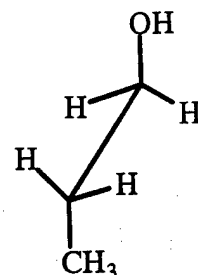
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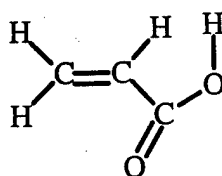
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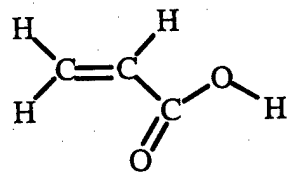
8c



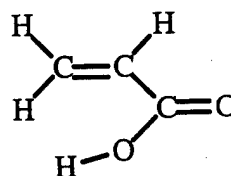
8d



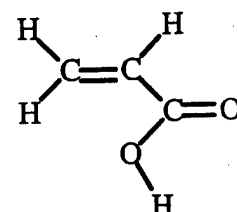
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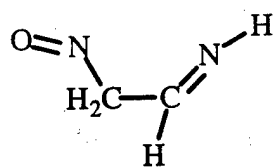
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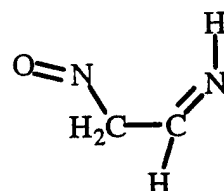
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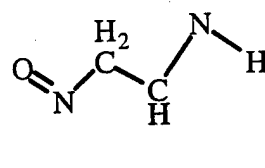
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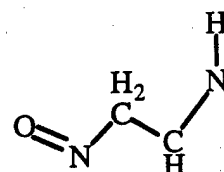
10a



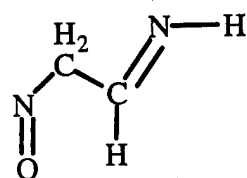
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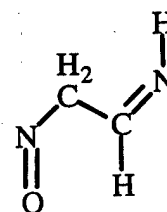
10c



10d



10e



10f